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# NUMERICAL METHODS FOR 2-DIMENSIONAL MODELLING

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The present status of MEMBRE, a fast computer code for calculating two-dimensional dopant redistribution during nonuniform oxide growth, is reviewed. Recent improvements in the code are outlined. A list of organizations that have requested and received copies of MEMBRE is given.

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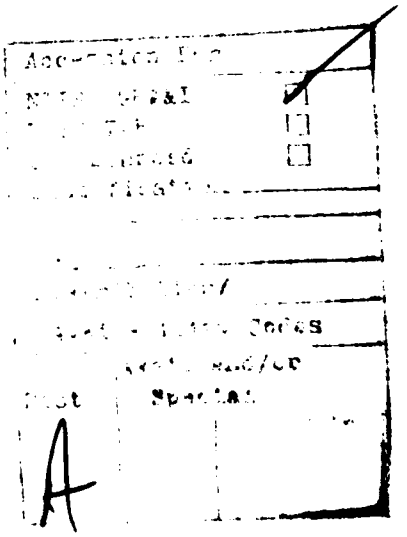
TABLE OF CONTENTS





# 1.0 SUMMARY

This document constitutes the final report under Contract MDA903-80-C-0498, DARPA Order No. 3984, on research in efficient numerical methods for two-dimensional VLSI process modeling. The major output of this work is embodied in the computer code MEMBRE (for Multidimensional Efficient Moving Boundary Redistribution) and the associated user's manual, which was published as the appendix to semi-annual technical report No. 3 under this contract. This code predicts the two-dimensional dopant profiles which evolve during oxidation and drive-in, including those effects arising from formation of the bird's beak oxide profile and from concentration dependence of the diffusivity at high doping levels. Typical CPU (central processing unit) times for a complete redistribution process, involving several thermal cycles, are found to range from two to ten minutes on the IBM 3033.

In the final phase of the contract, modifications have been introduced in the basic code to increase the speed of solution for the more difficult cases (e.g., arsenic drive-in). A factor of two reduction in CPU time was found to be achievable without deterioration in solution accuracy through the use of nonuniform spatial grids.

MEMBRE has been made available on tape to the U.S. integrated circuits community in the form of a FORTRAN program executable on the IBM 3033. It contains the basic input/output routines from Stanford's one-dimensional process code SUPREM, modified to deal with two-dimensional process data. Its capabilities have been described in presentations at two technical meetings[1,2] and in an article to appear in the new journal COMPEL.[3] Eight requests for the code from integrated circuit manufacturers and researchers in the U.S. have been processed to date.

## 1.1 Task Objectives

The overall objective of this program has been to develop fast and accurate methods for computer modeling of the two-dimensional spread of

dopants and other defects during VLSI circuit fabrication. Our goals for the first year were to demonstrate a fast algorithm for calculating nonlinear diffusion of a single dopant during nonuniform oxide growth, and to provide this algorithm in a form suitable for incorporation into a general process simulator such as Stanford's SUPREM. These goals have been accomplished.

The specific objectives for the second year included:

1. Effective transfer of the basic algorithm to the integrated circuits community;

2. Extension of the code to treat multiple interacting species and three-dimensional redistribution; and

3. Exploration of the computational requirements posed by better physical models for the underlying processes of chemical reaction and defect generation and migration.

## 1.2 Technical Problem

The fabrication of VLSI devices requires production of features of submicron size and separation. Electrical characteristics such as threshold and punchthrough voltages will be sensitive to dopant spread into critical areas adjacent to the original features. Experimental control of this spreading, without guidance from accurate computer modeling, will be costly, tedious, and time-consuming. However, the use of standard numerical methods to achieve an adequate modeling capability is also costly and time-consuming. One should therefore seek advanced methods, drawn from areas such as fluid dynamics, where considerable effort and ingenuity have been expended in recent years to develop fast and accurate solvers for the characterization of multidimensional, time-dependent phenomena.

## 1.3 General Methodology

Based on our own ongoing research in computational nonlinear aerodynamics, we identified several promising approaches to the development of a fast solver for two-dimensional diffusion problems. After a preliminary screening, a few of these were selected for adaptation to the problem of dopant spread during oxidation or annealing. These algorithms were tested for speed and accuracy on the problem of nonlinear dopant diffusion into the channel region of a MOSFET, as well as on simpler problems for which the actual dopant profiles could be accurately obtained by other means.

The algorithm finally selected for further development provided not only exceptional speed, but also a natural extendability to interacting defect species and three-dimensional diffusion.

## 1.4 Technical Results

The specific improvements in MEMBRE accomplished during the final phase of this contract are described in Section 2 of this report. They include a technique for clustering grid points in regions of large spatial gradient (nonuniform gridding) and optimization of the code for execution on the Cray-1 computer, which has become generally available for engineering calculations during the past year.

## 1.5 Important Findings and Conclusions

We restate here the conclusions presented in semiannual technical report No. 3, as they provide an appropriate summary for the total contract effort. The speed with which MEMBRE can predict the effect of process conditions on 2-D dopant spread should make the code a useful tool in the interactive design of VLSI fabrication processes. Many of the most common features in MOSFET fabrication fall within the modeling capabilities of the present code. However, it should be remembered that this code is intended only as a demonstration of 2-D modeling capabilities. It is not a complete process simulator, nor has it been optimized for its present use. Rather, it is pre-

sented in a format designed to encourage adaptation and extension. The basic algorithm, whose software implementation is included in MEMBRE, is capable of solving problems of much greater complexity.

## 1.6 Implications for Further Research

The development of efficient numerical methods for the various phases of VLSI design is an important goal that is partially realized in MEMBRE. Achieving comparable speed in the computation of device electrical characteristics and circuit transient behavior appears more difficult, based on the available numerical algorithms. Researchers active in this area may benefit from an investigation of the applicability of the ideas underlying the fast solver in MEMBRE to their problems.

## 2.0 PROGRESS ON TWO-DIMENSIONAL PROCESS MODELING

Two major developments were accomplished during the last reporting period: (1) The computer code MEMBRE was modified to allow for a variable spatial grid, (2) the program was vectorized and converted for execution on the Cray-1 computer. The variable grid feature is very important for the redistribution of arsenic implants, which usually have large gradients over short distances.

The computational rectangle is now covered by a nonuniform, arbitrary grid with coordinates $(\xi_i, \eta_j)$. Spatial derivatives are discretized using the following approximations:

$$\frac{\partial N_{ij}}{\partial \xi} \approx \frac{N_{i+1,j} - N_{i-1,j}}{\xi_{i+1} - \xi_{i-1}}$$

$$\frac{\partial N_{ij}}{\partial \eta} \approx \frac{N_{i,j+1} - N_{i,j-1}}{\eta_{j+1} - \eta_{j-1}}$$

$$\frac{\partial}{\partial \xi}\left[D(N)\frac{\partial N}{\partial \xi}\right]_{ij} \approx \frac{2}{\xi_{i+1} - \xi_{i-1}}\left[\frac{N_{i+1,j} - N_{ij}}{\xi_{i+1} - \xi_i} D_{i+1/2,j} - \frac{N_{ij} - N_{i-1,j}}{\xi_i - \xi_{i-1}} D_{i-1/2,j}\right]$$

$$\frac{\partial}{\partial \eta}\left[D(N)\frac{\partial N}{\partial \eta}\right]_{ij} \approx \frac{2}{\eta_{j+1} - \eta_{j-1}}\left[\frac{N_{i,j+1} - N_{ij}}{\eta_{j+1} - \eta_j} D_{i,j+1/2} - \frac{N_{ij} - N_{i,j-1}}{\eta_j - \eta_{j-1}} D_{i,j-1/2}\right]$$

$$\frac{\partial}{\partial \eta}\left[D(N)\frac{\partial N}{\partial \xi}\right]_{ij} \approx \left[\frac{D_{i,j+1}(N_{i+1,j+1} - N_{i-1,j+1}) - D_{i,j-1}(N_{i+1,j-1} - N_{i-1,j-1})}{(\eta_{j+1} - \eta_{j-1})(\xi_{i+1} - \xi_{i-1})}\right]$$

where $N_{ij} = N(\xi_i,\eta_j,\tau)$, $D_{i\pm1/2,j} = D[(N_{i\pm1,j} + N_{ij})/2]$, $D_{ij} = D(N_{ij})$, etc. As before, D(N) represents a nonlinear concentration-dependent diffusivity. In order to incorporate the above difference equations into the original uniform code, modifications were required in the following subroutines: ASET, DIFFUN, INIT, LDNXI1, LOADDX, LOADDY, LOADJX, LOADJY, LOADNX, LODNYX, MAIN, OUTPT, and UFCT. Much of the symmetry present in the uniform grid code is no longer available; however, some computational savings may still be made. For example, if the FORTRAN variables DSAVE(I) and XISEP(I) represent

$$\text{DSAVE(I)} = \frac{N_{ij} - N_{i-1,j}}{\xi_i - \xi_{i-1}} D_{i-1/2,j}$$

and

$$\text{XISEP(I)} = 2/(\xi_{i+1} - \xi_{i-1})$$

for any fixed j, then

$$\frac{\partial}{\partial\xi}\left[D(N)\frac{\partial N}{\partial\xi}\right]_{ij} \approx \text{XISEP(I)} * (\text{DSAVE(I+1)} - \text{DSAVE(I)})$$

Most of the algorithms in MEMBRE vectorized automatically when using the Cray-1 compiler. However, two subroutines, LOADDX and LOADDY, make millions of calls to the external diffusivity function D(N). If this function is included as a statement function in LOADDX and LOADDY, a factor of two improvement on execution can be obtained. Below are the new listings of these subroutines on the Cray-1 for the nonuniform code.

Presently, the variable grid is loaded using FORTRAN statements in the MAIN program. Eventually, the SUPREM input subroutines will be modified to allow for a variable grid input from a new GRID card.

```
      SUBROUTINE LOADDX (J,Y,DSAVE)
C     THIS SUBROUTINE COMPUTES THE DISCRETIZED DIFFERENCE EQUATION IN
C     THE X-DIRECTION USING THE METHOD OF LINES
      IMPLICIT REAL*8(A-H,O-Z)
      COMMON/PARM1/NX,NXP1,NY,NYP1,NXM1,JB1,JB2,JB1P1,JB2M1
      COMMON/PARM2/RDX2,RDY2,RHDX2,RHDY2,R2DX,R4DXDY,R2DY
      COMMON/PARM3/BETA,DBETA1,DBETA2,DBETA3,NI,HALFNI
      COMMON/SRDX2/SRDX2(1)
      DIMENSION DSAVE(1),Y(1)
      D(A,B) = DBETA1*(1.0+BETA*(A+B))*(1.0+A/B)
      ICOL = (J-1)*NX
      DO 10 I = 2,NX
      ISUB = ICOL+1
      ISUBM1 = ISUB-1
      YH = 0.5D0*(Y(ISUB)+Y(ISUBM1))
      ALPHA = HALFNI*YH
      ALPHA = CVMGT(0.0,ALPHA,ALPHA.LT.0.0)
      TERM = SQRT(ALPHA*ALPHA+1.0)
      DSAVE(I) = SRDX2(I)*D(ALPHA,TERM)*(Y(ISUB)-(ISUBM1))
   10 CONTINUE
      DSAVE(1) = -DSAVE(2)
      DSAVE(NXP1) = -DSAVE(NX)
      RETURN
      END
```

```
      SUBROUTINE LOADDY(I,Y,DSAVE)
C     THIS SUBROUTINE COMPUTES THE DISCRETIZED DIFFERENCE EQUATION IN
C     THE Y-DIRECTION USING THE METHOD OF LINES
      IMPLICIT REAL*(A-H,O-Z)
      COMMON/PARM1/NX,NXP1,NY,NYP1,NXM1,JB1,JB2,JB1P1,JB2M1
      COMMON/PARM2/RDX2,RDY2,RHDX2,RHDY2,R2DX,R4DXDY,R2DY
      COMMON/PARM3/BETA,DBETA1,DBETA2,DBETA3,NI,HALFNI
      COMMON/SRDY2/SRDY2(1)
      DIMENSION DSAVE(1),Y(1)
      D(A,B) = DBETA1*(1.0+BETA*(A+B))*(1.0+A/B)
      IC1 = I-NX
      IC2 = IC1-NX
      DO 10 J = 2,NY
      YH = 5DO*(Y(NX*J+IC1)+Y(NX*J+IC2))
      ALPHA = HALFNI*YH
      ALPHA = CVMGT(0.0,ALPHA,ALPHA.LT.0.0)
      TERM = SQRT(ALPHA*ALPHA+1.0)
      DSAVE(J) = SRDY2(J)*D(ALPHA,TERM)*(Y(NX*J+IC1) - Y(NX*J+IC2))
   10 CONTINUE
      DSAVE(1) = -DSAVE(2)
      DSAVE(NYP1) = -DSAVE(NY)
      RETURN
      END
```

Two cases were studied to determine the effect of the variable grid on accuracy and execution time on the Cray-1.

Case 1. Redistribution of Boron Field Implant

This case consists of the development of a bird's beak. The silicon slab is 2 μm × 3 μm. In the uniform case $\Delta\xi = \Delta\eta = 0.05$ μm which produces a spatial grid of 41 × 61 points. A 150 KeV boron implant of dose $2.5 \times 10^{12}$ $cm^{-2}$ is simulated. The first cycle consists of oxidation at a temperature of 1000°C for 20 minutes in nitrogen. This is followed by a nonuniformly moving boundary cycle for 160 minutes in steam at 1000°C. The actual SUPREM like input data is listed below for the uniform grid case.

```
1     TITL  BORON FIELD IMPLANT, E-NMOS
2     GRID DYSI=0.05,DPTH=0.05,YMAX=2,DELY=0.05,YLMX=3
3     SUBS  ORNT=100,ELEM=+,CONC=5E14
4     COMM  STARTING OXIDE THICKNESS OF 0.005 UM
5     STEP  TYPE=DEPO,TIME=1,GRTE=0.005
6     PLOT TOTL=Y
7     PRINT TOTL=Y,HEAD=Y
8     COMM  150 KEV BORON IMPLANT
9     STEP  TYPE=IMPL,ELEM=B,DOSE=2.5E12,AKEV=150,YDEV=0.148,
10    +     YWIN=1.
11    PLOT TOTL=N
12    COMM  FIELD OXIDATION
13    STEP  TYPE=OXID,TEMP=1000,TIME=20,MODL=NITØ
14    STEP  TYPE=OXID,TEMP=1000,TIME=160,MODL=WETØ,RATO=0.3333,
15    +     YPEN=0.075
16    END
```

The 27 × 44 nonuniform grid for this problem is as follows:

XI GRID

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 0.0000 | 0.0500 | 0.1000 | 0.1500 | 0.2000 | 0.2500 | 0.3000 | 0.3500 |
| 0.4000 | 0.4500 | 0.5000 | 0.5500 | 0.6000 | 0.6500 | 0.7000 | 0.7500 |
| 0.8000 | 0.8500 | 0.9000 | 0.9500 | 1.0000 | 1.1000 | 1.2000 | 1.4000 |
| 1.6000 | 1.8000 | 2.0000 | | | | | |

ETA GRID

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 0.0000 | 0.0500 | 0.1000 | 0.1500 | 0.2000 | 0.2500 | 0.3000 | 0.3500 |
| 0.4000 | 0.4500 | 0.5000 | 0.5500 | 0.6000 | 0.6500 | 0.7000 | 0.7500 |
| 0.8000 | 0.8500 | 0.9000 | 0.9500 | 1.0000 | 1.0500 | 1.1000 | 1.1500 |
| 1.2000 | 1.2500 | 1.3000 | 1.3500 | 1.4000 | 1.4500 | 1.5000 | 1.5500 |
| 1.6000 | 1.6500 | 1.7000 | 1.7500 | 1.8000 | 1.9000 | 2.0000 | 2.2000 |
| 2.4000 | 2.6000 | 2.8000 | 3.0000 | | | | |

Although accuracy is essentially the same for both grids in all areas of critical interest, CPU time is much better for the variable grid - 10.365 seconds versus 18.902 seconds. Using a cruder nonuniform grid would yield a further improvement in speed, but accuracy would begin to deteriorate.

Case 2. Redistribution of Arsenic Source/Drain Implant

This case consists of the oxidation for 40 minutes of a very steep 40 KeV arsenic profile having a projected range ($R_p$) of 0.0265 and projected and lateral standard deviations of 0.0099 and 0.0103, respectively. An explosive type diffusion is characteristic of such problems, and a very fine uniform grid of 51 × 61 on a silicon slab of 1.25 μm × 1.5 μm was required to maintain accuracy. The initial data is listed below:

```
1     TITL  ARSENIC SOURCE/DRAIN IMPLANT, E-NMOS
2     GRID  DYSI = 0.025, DPTH = 0.025, YMAX = 1.25, DELY = 0.025,
      +     YLMX = 1.5
3     SUBS  ORNT = 100, ELEM =+, CONC = 5E14
4     PLOT  TOTL = Y, CMIN = 14, NDEC = 4, WIND = 2
5     PRINT TOTL = Y, HEAD = Y
6     COMM  40 KEV ARSENIC IMPLANT
7     STEP  TYPE = IMPL, ELEM = AS, DOSE = 1E16, RANG = 0.0265, STDV
8     +     = 0.0099, YWIN = 0.5, YDEV = 0.0103
9     COMM  ARGON ANNEAL
10    STEP  TYPE = OXID, TEMP = 1000, TIME = 40, MODL = NITØ
11    END
```

The following 33 × 47 nonuniform grid produced the same quality of accuracy:

XI GRID

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 0.0000 | 0.0250 | 0.0500 | 0.0750 | 0.1000 | 0.1250 | 0.1500 | 0.1750 |
| 0.2000 | 0.2250 | 0.2500 | 0.2750 | 0.3000 | 0.3250 | 0.3500 | 0.3750 |
| 0.4000 | 0.4250 | 0.4500 | 0.4750 | 0.5000 | 0.5250 | 0.5500 | 0.5750 |
| 0.6000 | 0.6500 | 0.7000 | 0.7500 | 0.8500 | 0.9500 | 1.0500 | 1.1500 |
| 1.2500 | | | | | | | |

ETA GRID

| | | | | | | | |
|---|---|---|---|---|---|---|---|
| 0.0000 | 0.0250 | 0.0500 | 0.0750 | 0.1000 | 0.1250 | 0.1500 | 0.1750 |
| 0.2000 | 0.2250 | 0.2500 | 0.2750 | 0.3000 | 0.3250 | 0.3500 | 0.3750 |
| 0.4000 | 0.4250 | 0.4500 | 0.4750 | 0.5000 | 0.5250 | 0.5500 | 0.5750 |
| 0.6000 | 0.6250 | 0.6500 | 0.6750 | 0.7000 | 0.7250 | 0.7500 | 0.7750 |
| 0.8000 | 0.8250 | 0.8500 | 0.8750 | 0.9000 | 0.9250 | 0.9500 | 0.9750 |
| 1.000 | 1.0500 | 1.1000 | 1.2000 | 1.3000 | 1.4000 | 1.5000 | |

Computation times were 20.091 seconds on the 33 × 47 grid and 36.008 seconds on the 51 × 61 uniform grid. These results indicate that a factor of two improvement in computation time can be achieved when using a nonuniform grid. In addition, the Cray-1 is about 13 times faster than the IBM 3033. Thus, a 26 fold improvement in computer execution time was achieved over our previously reported data.

## 3.0 PRESENTATIONS AND PUBLICATIONS

1. W. D. Murphy, W. F. Hall, and C. D. Maldonado, "Efficient Numerical Solution of Two-Dimensional Nonlinear Diffusion Equations with Nonuniformly Moving Boundaries: A Versatile Tool for VLSI Process Modeling," presented at the Second International Conference on the Numerical Analysis of Semiconductor Devices and Integrated Circuits, NASECODE II, June 17-19, 1981, in Dublin, Ireland, Also published by Boole Press, Dublin, as part of the proceedings of that conference (pp. 249-253).

2. C. D. Maldonado, W. F. Hall, W. D. Murphy, and S. A. Louie, "2D Process Modeling and Simulation for VLSI Design," presented at the 1981 Symposium on VLSI Technology, September 9-11, 1981, in Maui, Hawaii.

3. W. D. Murphy, W. F. Hall, C. D. Maldonado, and S. A. Louie, "MEMBRE: An Efficient Two-dimensional Process Code for VLSI," to appear in COMPEL

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